Data need for JWST
(...and E-ELT, ALMA/SKA/SPICA)

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# Summary

## Atomic

- $T_e$, $n_e$, abundances
  - TIPbase project. Overall happy with data in hand
- $\Omega_{\text{col}}$ for [NeV], resolve differences (e.g. [SIII], [NII])
- Old values, renew?

## Molecular

- Excitation conditions
  - UMIST, CDMS, JPL
- Collisional rates for CH$^+$ with $H_2/e^-$ and OH with $H_2$
- Fullerenes: discrepancy relative strengths of C$_{60}$!

## PAHs/HAC/…

- Dust evolution, star formation tracers
  - NASA Ames, Jena db
- Molecular physics of large aromatics
- Spectra of carbonaceous dust (HAC/soot…)

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**JWST**

**Herschel, ALMA, SKA, SPICA, JWST**

**JWST, E-ELT**
Atomic data

- Fundamental to all methods of measuring $T_e$, $n_e$, and abundances in gaseous nebulae
  - H, He recombination lines
  - Collisionally excited lines for heavy elements

IR lines: accurate abundance determination
- ISO/Spitzer: Local/nearby galaxies
- JWST: across and distant galaxies (diagnostic)

(A, $\Omega_{\text{col}}$)
Atomic data

- TIPbase from IRON project: easy, relevant T ~ 3,000-20,000 K. Also CHIANTI

- Collisional strengths:
  - [NeV]) observations and theory do not agree. Some ions have different values (e.g. [SIII], [NII])
  - Uncertainties not clear in some cases, also some data are 20yr old…

- We use effective collisional strengths (MB). And if non-electron energy distribution?

- Could this explain difference between observations/theory, and difference between collisional excited and recombination lines?

C, N, O, Ne, S, Ar, Mg, Fe (Cl) — II, III, IV, V, VI — 5 level
Molecules: OH, CH⁺

- Key molecules tracing warm & dense phase of the ISM, also observed in diffuse ISM
- Important to constrain their formation and excitation!
- We use codes (Meudon, RADEX) which take UMIST, CDMS, JPL databases (CASSIS)
- **We need** collision rates: CH⁺ with H₂ and e⁻, and OH with e⁻ for 10 < T < 2,000 K
- Now detected extragalactic environments!

Parikka et al. (2015)
Extragalactic

Growth area for:
- ALMA
- SKA
- SPICA...

Rangwala et al. (2011)

OH, OH+, CH+, H2O, HCN, HNC, CS, HF...
Fullerenes

Cami, Bernard-Salas et al. (2010, Science)
What is going on?

- We need reliable relative strength of the C$_{60}$ bands
- Also, what is the effect of $^{13}$C in spectra?
UIB - (PAHs, HAC, …)

- Rich (unidentified) chemistry in evolved stars
- PAHs ubiquitous in the Universe, vary in profile relative strength, peak position
- HAC: key element in linking these features

Peeters et al. (2003)  
Bernard-Salas et al. (2012)

JWST spatially resolved studies of mid-IR in proto-planetary discs, and detect PAHs z~3.7, evolved stars up to the Virgo cluster
PAHs

- Direct measurements from spectra or decomposition methods

PAHFIT Smith et al. (2007)

- Best use spectral fits based on experimental or computational data (e.g. PAH, NASA-Ames)

Joblin et al. (2008)
• Need experiments for larger PAHs (>40) and >3+ charge states for large PAHs
• Molecular physics of large aromatics (high energy, anharmonicities, fragmentation)
HAC, soot,…

• Use Jena database, Menella, Zubko…

• Optical properties of c-material at longer wavelength (>6μm) not well characterised

• We do not have a good idea of how soot, clusters look like

• E-ELT will offer to study the aliphatic-aromatic components in the 3μm region

- Ideally we want gas-phase optical properties of PAHs, HAC
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- Different \(\Omega_{\text{col}}\) for some ions e.g. [SIII], [NII], [NeV]
- Old values, uncertainties?

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- Excitation conditions
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**JWST**

**ALMA, SKA, JWST, SPICA**

**JWST, E-ELT**